

cycloalkyl, C₂-C₁₀ alkenyl, and C₂-C₁₀ alkynyl, wherein n is 0, 1, 2, or 3, and the (CH₂)_nAr, (CH₂)_nheteroaryl, alkyl, cycloalkyl, alkenyl, and alkynyl groups are optionally substituted by up to 5 groups selected from NR⁴R⁵, N⁷(O)R⁴R⁵, N⁴R⁵R⁶Y⁷, alkyl, phenyl, substituted phenyl, (CH₂)_nheteroaryl, hydroxy, alkoxy, phenoxy, thiol, thioalkyl, halo, COR⁴, CO₂R⁴, CONR⁴R⁵, SO₂NR⁴R⁵, SO₃R⁴, PO₃R⁴, aldehyde, nitrile, nitro, heteroaryloxy,

OR⁵ | T(CH₂)_mQR⁴, T(CH₂)_mC-(CH₂)_mQR⁴, | | |

 $C(O)T(CH_2)_mQR^4$, $NHC(O)T(CH_2)_mQR^4$, $T(CH_2)_mC(O)NR^4NR^5$, or $T(CH_2)_mCO_2R^4$ wherein each m is independently 1-6, T is O, S, NR^4 , $N^+(O)R^4$, $N^+R^4R^6Y^-$, or QR^4R^5 , and Q is O, S, NR^5 , $N^+(O)R^5$ or $N^+R^5R^6Y^-$;

and additionally alkyl, alkenyl and alkynyl can be further substituted with one to three cycloalkyl groups,

when the dotted line is present, R^3 is absent; otherwise R^3 has the meanings of R^2 , wherein R^2 is as defined above, as well as OH, NR^4R^5 , $COOR^4$, OR^4 , $CONR^4R^5$, $SO_2NR^4R^5$, SO_3R^4 , PO_3R^4 , $T(CH_2)_mQR^4$,

OR⁵ | T(CH₂)_mC-(CH₂)_mQR⁴, | | |

wherein T and Q are as defined above;

 R^4 and R^5 are each independently selected from the group consisting of hydrogen, C_1 - C_6 alkyl, substituted alkyl, C_2 - C_6 alkenyl, C_2 - C_6 alkynyl, $N(C_1$ - C_6 alkyl)_{1 or 2}, $(CH_2)_n$ Ar, C_3 - C_{10} cycloalkyl, heterocyclyl, and

heteroaryl, or R⁴ and R⁵ together with the nitrogen to which they are attached optionally form a ring having 3 to 7 carbon atoms and said ring optionally contains 1, 2, or 3 heteroatoms selected from the group consisting of nitrogen, substituted nitrogen, oxygen, and sulfur;

when R⁴ and R⁵ together with the nitrogen to which they are attached form a ring, the said ring is optionally substituted by 1 to 3 groups selected from OH,



OR⁴, NR⁴R⁵, (CH₂)_mOR⁴, (CH₂)_mNR⁴R⁵, T-(CH₂)_mQR₄, CO-T-(CH₂)_mQR⁴, NH(CO)T(CH₂)_mQR⁴, T-(CH₂)_mCO₂R⁴, or T(CH₂)_mCONR⁴R⁵;

R⁶ is alkyl;

 R^8 and R^9 independently are H, NR^4R^5 , $N^+(O)R^4R^5$, $N^+R^4R^5R^6Y^-$, COR^4 , CO_2R^4 , $CONR^4R^5$, $SO_2NR^4R^5$, SO_3R^4 , PO_3R^4 , CN or nitro;

when the dotted line is absent, R⁹ can additionally be = NOH,

= NOalkyl, =NOalkenyl, =NOalkynyl or =NOcycloalkyl; and

Y is a halo counter-ion;

with the proviso that: (a) when R^8 and R^9 are both hydrogen, W is NH, R^1 is hydrogen and X is NR^{10} , then R^{10} is neither unsubstituted (C_1 - C_{10}) alkyl, unsubstituted (C_1 - C_{10}) alkenyl nor unsubstituted (C_1 - C_{10}) alkynyl;

- (b) when R^8 or R^9 is NR^4R^5 , $N^4(O)R^4R^5$, or $N^7R^4R^5R^6Y^7$, then one or more of R^4 , R^5 and R^6 must be, independent of the nitrogen to which said one or more R^4 , R^5 and R^6 are attached, heterocyclic or heteroaryl; and
- (c) when R⁸ or R⁹ is COR⁴, CO₂R⁴, CONR⁴R⁵, SO₂NR⁴R⁵, SO₃R⁴ or PO₃R⁴, then one or more of R⁴, R⁵ and R⁶ must be, independent of the nitrogen to which said one or more R⁴, R⁵ and R⁶ are attached, (CH₂)_naryl wherein n is zero, 1, 2 or 3, heterocyclic or heteroaryl;
- (d) when X is S and W is NH, then at least one of R1, R2, R3, R8 and R9 is other than H or C₁-C₃ alkvl
- 55. A compound of Claim 54, wherein W is NH, and R⁸ and R⁹ both are hydrogen.



$$R^{1} - N \qquad N \qquad N \qquad 0$$

$$R^{2}$$

wherein:

R¹ and R² independently are hydrogen, C₁-C₁₀ alkyl, (CH₂)_nAr, (CH₂)_nheteroaryl, C₃-C₁₀ cycloalkyl, or (CH₂)_n heterocyclyl, wherein n is 0, 1, 2 or 3, and the (CH₂)_nAr, (CH₂)_nheteroaryl, alkyl, cycloalkyl and (CH₂)_n heterocyclyl groups are optionally substituted by up to 5 groups selected from NR⁴R⁵, N⁺(O)R⁴R⁵, N⁺R⁴R⁵R⁶Y⁻, alkyl, phenyl, substituted phenyl, (CH₂)_nheteroaryl, hydroxy, alkoxy, phenoxy, thiol, thioalkyl, halo, COR⁴, CO₂R⁴, CONR⁴R⁵, SO₂NR⁴R⁵, SO₃R⁴, PO₃R⁴, aldehyde, nitrile, nitro, heteroaryloxy, T(CH₂)_mQR⁴,

 $C(O)T(CH_2)_mQR^4$,

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NHC(O)T(CH₂)_mQR⁴, T(CH₂)_mC(O)NR⁴NR⁵, or T(CH₂)_mCO₂R⁴ wherein each m is independently 1-6, T is O, S, NR⁴, N⁺(O)R⁴, N⁺R⁴R⁶Y⁻, or CR⁴R⁵, and Q is O, S, NR⁵, N⁺(O)R⁵, or N⁺R⁵R⁶Y⁻; R³ has the meanings of R², wherein R² is as defined above, as well as OH, NR⁴R⁵, COOR⁴, OR⁴, CONR⁴R⁵, SO₂NR⁴R⁵, SO₃R⁴, PO₃R⁴,

OR⁵
|
$$T(CH_2)_mQR^4$$
, $T(CH_2)_mC$ -(CH_2) $_mQR^4$,
|
H

wherein T and Q are as defined above;

R⁴ and R⁵ are each independently selected from the group consisting of hydrogen, C₁-C₆ alkyl, substituted alkyl, C₂-C₆ alkenyl, C₂-C₆ alkynyl, N(C₁-C₆alkyl)₁ or 2, (CH₂)_nAr, C₃-C₁₀ cycloalkyl, heterocyclyl, and

heteroaryl, or R⁴ and R⁵ together with the nitrogen to which they are attached optionally form a ring having 3 to 7 carbon atoms and said ring optionally contains 1, 2, or 3 heteroatoms selected from the group consisting of nitrogen, substituted nitrogen, exygen, and sulfur;

when R⁴ and R⁵ together with the nitrogen to which they are attached form a ring, the said ring is optionally substituted by 1 to 3 groups selected from OH, OR⁴, NR⁴R⁵, (CH₂)_mOR⁴, (CH₂)_mNR⁴R⁵, T-(CH₂)_mQR₄,

CO-T-(CH₂)_mQR⁴, NH(CO)T(CH₂)_mQR⁴, T-(CH₂)_mCO₂R⁴, or

 $T(CH_2)_m CONR^4R^5$;

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R⁶ is alkyl; and

Y is a halo counter-ion.

57. A compound of Claim 54 wherein W is S, SO, or SO₂.

58. A pharmaceutical formulation comprising a compound of compound of Formula I

or a pharmaceutically acceptable salk thereof, wherein:

the dotted line represents an optional double bond; W is NH, S, SO, or SO₂;

X is either O, S, or NR¹⁰;

R¹, R², and R¹⁰ are independently selected from the group consisting of H, (CH₂)_nAr, COR⁴, (CH₂)_nheteroaryl, (CH₂)_nheterocyclyl, C₁-C₁₀ alkyl, C₃-C₁₀ cycloalkyl, C₂-C₁₀ alkenyl, and C₂-C₁₀ alkynyl, wherein n is 0, 1, 2, or 3, and the (CH₂)_nAr, (CH₂)_nheteroaryl, alkyl, cycloalkyl, alkenyl, and alkynyl groups are optionally substituted by up to 5 groups selected from NR⁴R⁵, N⁺(O)R⁴R⁵, N⁺(O)R⁴R⁵, N⁺(Ar⁵R⁶Y⁻, alkyl, phenyl, substituted phenyl, (CH₂)_nheteroaryl, hydroxy,

alkoxy, phenoxy, thiol, thioalkyl, halo, COR⁴, CO₂R⁴, CONR⁴R⁵, SO₂NR⁴R⁵, SO₃R⁴, PO₃R⁴, aldehyde, nitrile, nitro,

heteroaryloxy, $T(CH_2)_mQR^4$,

OR⁵ | T(CH₂)_mC-(CH₂)_mQR⁴, | | |

C(O)T(CH₂)_mQR⁴, NHC(O)T(CH₂)_mQR⁴, T(CH₂)_mC(O)NR⁴NR⁵, or T(CH₂)_mCO₂R⁴ wherein each m is independently 1-6, T is O, S, NR⁴, N⁺(O)R⁴, N⁺R⁴R⁶Y⁻, or CR⁴R⁵, and Q is O, S, NR⁵, N⁺(O)R⁵ or N⁺R⁵R⁶Y⁻;

and additionally alkyl, alkenyl and alkynyl can be further substituted with one to three cycloalkyl groups,

when the dotted line is present, R³ is absent; otherwise R³ has the meanings of R², wherein R² is as defined above, as well as OH, NR⁴R⁵, COOR⁴, OR⁴, CONR⁴R⁵, SO₂NR⁴R⁵, SO₃R⁴, PO₃R⁴,

OR⁵ T(CH₂)_mQR⁴, T(CH₂)_mC-(CH₂)_mQR⁴,

wherein T and Q are as defined above;

R⁴ and R⁵ are each independently selected from the group consisting of hydrogen, C₁-C₆ alkyl, substituted alkyl, C₂-C₆ alkenyl, C₂-C₆ alkynyl, N(C₁-C₆alkyl)_{1 or 2}, (CH₂)_nAr, C₃-C₁₀ cycloalkyl, heterocyclyl, and heteroaryl, or R⁴ and R⁵ together with the nitrogen to which they are attached optionally form a ring having 3 to 7 carbon atoms and said ring optionally



contains 1, 2, or 3 heteroatoms selected from the group consisting of nitrogen, substituted nitrogen, oxygen, and sulfur;

when R⁴ and R⁵ together with the nitrogen to which they are attached form a ring, the said ring is optionally substituted by 1 to 3 groups selected from OH, OR⁴, NR⁴R⁵, (CH₂)_mOR⁴, (CH₂)_mNR⁴R⁵, T-(CH₂)_mQR₄,

CO-T-(CH₂)_mQR⁴, NH(CO)T(CH₂)_mQR⁴, T-(CH₂)_mCO₂R⁴, or $T(CH_2)_mCONR^4R^5$;

R6 is alkyl;

R⁸ and R⁹ independently are H, NR⁴R⁵, N⁺(O)R⁴R⁵, N⁺R⁴R⁵R⁶Y⁻, COR⁴, CO₂R⁴, CONR⁴R⁵, SO₂NR⁴R⁵, SO₃R⁴, PO₃R⁴, CN or nitro;

when the dotted line is absent, R⁹ can additionally be = NOH,

= NOalkyl, =NOalkenyl, =NOalkynyl or =NOcycloalkyl; and

Y is a halo counter-ion;

with the proviso that: (a) when R^8 and R^9 are both hydrogen, W is NH, R^1 is hydrogen and X is NR^{10} , then R^{10} is neither unsubstituted (C_1 - C_{10}) alkyl, unsubstituted (C_1 - C_{10}) alkynyl; and

- (b) when R⁸ or R⁹ is NR⁴R⁵, N⁴(O)R⁴R⁵, N⁴R⁵R⁶Y⁷, COR⁴, CO₂R⁴, CONR⁴R⁵, SO₂NR⁴R⁵, SO₃R⁴ or PO₃R⁴, then one or more of R⁴, R⁵ and R⁶ must be, independent of the nitrogen to which said one or more of R⁴, R⁵ and R⁶ is attached, (CH₂)_naryl wherein n is zero, 1, 2, or 3, heterocyclic or heteroaryl;
- (c) when X is S and W is NH, then at least one of R1, R2, R3, R8 and R9 is other than H or C1-C3 alkyl;

in combination with a pharmaceutically acceptable carrier, diluent, or excipient.

59. A pharmaceutical formulation comprising a compound of Claim 56 in combination with a pharmaceutically acceptable carrier, diluent or excipient. - -